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Intersubband Transitions in Quantum-Well Heterostructures with Delta-Doped Barriers

by

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A single quantum well doped by a negative delta-function potential (δ-potential) in the barrier regions is analyzed in terms of the optical transitions inbetween subbands. The first two states of the quantum well do not change at all as a function of the strength of the δ-potential up to a certain value, whereas the third one gets lowered almost exponentially. An important point is that the δ-potential brings a state from the continuum to the bound region. There is a range of the strength of the δ-potential during which the transition energy from the first to second state decreases rapidly, and at a certain strength the first and second states disappear, and the third and fourth, which have been brought from the continuum, take their places. The oscillator strengths of the allowed transitions have a kind of oscillatory behavior in that range.

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Intersubband transitions in quantum-well heterostructures with delta-doped barriers

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A single quantum well doped by a negative delta-function potential (δ-potential) in the barrier regions is analyzed in terms of the optical transitions in between subbands. The first two states of the quantum well do not change at all as a function of the strength of the δ-potenial up to a certain value, whereas the *third* one gets lowered almost exponentially. An important point is that the δ-potential brings a state from the continuum to the bound region. There is a range of the strength of the δ-potential during which the transition energy from the *first* to *second* state decreases rapidly, and at a certain strength the *first* and *second* states disappear, and the *third* and *fourth*, which have been brought from the continuum, take their places. The oscillator strengths of the allowed transitions have a kind of oscillatory behavior in that range.

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Artificially-fabricated semiconductor microstructures have been found to be very important for optical measurements and laser physics, and have been the subject of study for the last couple of decades because of their possible device applications and also because of their intrinsic simple physics. For modern day technologies, it is very easy to judiciously tailor any particular device to exhibit a given physical property, especially when the carriers are confined in a certain dimension, such as quantum-well wires and dots. In quantum wells, the allowed intersubband transition frequencies are generally on the order of infrared frequencies for moderate widths and heights of the wells. Intersubband and intrasubband transitions have been extensively studied experimently[1-3] and theoretically.[4-8] These studies involve a variety of III-V semiconductor heterostructures such as $GaAs$ and $Al_yGa_{1-y}As$, $InGaAS$ and InP, and $InGaAs$ and $InAlAs$. In most of these cases the barrier regions are doped randomly to populate the ground state, but in some cases it is also possible to populate the ground state optically.

Theoretically, a tailoring of intersubband transition energies was proposed by Trzeciakowski and McCombe[4] by growing a thin layer of $Al_yGa_{1-y}As$ with variable Al fraction. This extra barrier in the middle of the well alters the ground-state energy, with the energy of the first-excited state remaining essentially the same because of the nature of the wavefunction of this state which vanishes in the middle of the well for a symmetric quantum well. Since the wavefunction of the ground state is altered significantly, the oscillator strength decreases as the middle barrier height (Al fraction in $Al_yGa_{1-y}As$) increases.

A similar tailoring is also possible by doping the middle of the well by a positive delta-function potential (δ-potential)[5]. The epitaxial growth of the δ-potential is done by the growth-interruption technique.[9] In the process of growing the epitaxy layer, the donor or acceptor impurities could be grown randomly. These random impurities are very often the source of the carriers in such structures. However, the growth of the δ-potential could be achieved by depositing appropriate impurity atoms while suspending the deposition of epitaxy layers. By this technique a finite-width $\vee$ or $\wedge$-shaped δ-potentials of given

strength can be formed. A finite-width δ-potential means that Va is finite, with V and a individually also finite, where V and a are the depth or height and width (i.e. full width at half maximum) of the δ-potential, respectively.

In the present Letter, we propose a different kind of structure for tailoring of the intersubband transitions. Let us suppose a quantum well consists of $GaAs$ of width d and height V_0 with walls extending to infinity and made of $Al_yGa_{1-y}As$ material, which is doped randomly to provide enough electrons as carriers in the ground state. A negative δ-potential of strength, say δ, is doped at a_δ from both edges of the well. In the present calculation, we take the wavefunctions and their derivatives divided by the effective mass[10] to be continuoues at the boundaries. Although the epitaxial growth of the the δ-potentials gives a finite potential, we treat it as if it is infinite, meaning, $\Psi^+(a_\delta) = \Psi^-(a_\delta)$ and $\frac{\partial\Psi^+(a_\delta)}{\partial x} - \frac{\partial\Psi^-(a_\delta)}{\partial x} = \delta'\Psi^+(a_\delta)$. Here $\delta' = \frac{2m_b^*\delta}{\hbar^2}$, where δ is the strength of the δ-potential in eVÅ, m_b^* is the effective mass of the electrons in the barrier regions in which the negative δ-potential is grown, and the $\pm$ superscripts to Ψ refer to the values of the wavefunctions at the left and right of the δ-potential. The effective mass of the electrons is calculated based on the Al fraction in the $Al_yGa_{1-y}As$ layers.[11] x is the growth direction in which electrons are confined.

The eigenvalue condition for the δ-doped single quantum well described above is given by

$$\Theta(E) = 2\{X^2 - Y^2\}\cos(kd) + \{(X^2 + Y^2)Z^- + 2XYZ^+\}\sin(kd)\ . \qquad (1)$$

Here, $X = 2K + \delta'$, $Y = \delta'\exp(-2Ka_\delta)$, $Z^\pm = \{\frac{Km_w^*}{km_b^*} \pm \frac{km_b^*}{Km_w^*}$, $K = \sqrt{\frac{2m_b^*(V_0-E)}{\hbar^2}}$, and $k = \sqrt{\frac{2m_w^*E}{\hbar^2}}$. E is the energy of the electron and m_w^* is the effective mass of the electrons in the $GaAs$ layers.[11] Equation (1) is appropriate for calculating the stationary states of the quantum wells with negative or positive δ-doped structures in the barrier materials by finding the zeros the of the $\Theta(E)$, whereas the virtual (continuum) states of the structure are calculated with the help of transmission coefficients which are determined in the usual

manner. To calculate the virtual states, we consider the electrons to be moving in the $Al_yGa_{1-y}As$ medium except for the $GaAs$ layers with a potential of $-V_0$. The amplitude of the i-th state wavefunction $A^+_{a_\delta}$ in the region left of the δ-potential in the barrier left of the quantum well is given as

$$A^+_{a_\delta}(E_i) = -4K^2[\delta'^2 + 2\delta'\cos(ka)\{2K\cosh(2Ka_\delta) + \delta'\sinh(2Ka_\delta)\} + \sin(ka)\{2K\delta' Z^- \sinh(2Ka_\delta) + \delta'^2 Z^+ \cosh(2Ka_\delta) - Z^-(2K^2 - \delta'^2)\}].^{-1}(2)$$

Here E_i is the eigenvalue of the the i-th state and K and k are calculated for $E = E_i$. The other coefficients can be calculated by matrix multiplications which involve an algebraic exercise and are not given here for brevity. The wavefunctions of all the states are normalized to unity,

$$\int_{-b}^{b} dx|\Psi(x)|^2 = 1 \ , \tag{3}$$

where $b = 3(d/2 + a_\delta)$, which is infinity in the practical sense since the wavefunctions are essentially zero beyond -b and b. The dipole matrix elements for the transition from the state i to the state j is expressed as

$$z(i \leftrightarrow j) = \int_{-b}^{b} dx\Psi^*_j(x)\ x\ \Psi_i(x) \ . \tag{4}$$

Here $\Psi^*_j(x)$ is the complex conjugate of the wavefunction for the state j. We should point out that the complex conjugate of a wavefunction for the cases studied here is immaterial since these states are stationary. However, it may result in complex dipole moments for the transitions between stationary and virtual states. The oscillator strength describing the transition $i \leftrightarrow j$ is defined as

$$f(i \leftrightarrow j) = \frac{2m_0\omega_{ij}}{\hbar}|z(i \leftrightarrow j)|^2 \ , \tag{5}$$

where $\omega_{ij} = \frac{|E_i - E_j|}{\hbar}$ is the transition frequency between the states i and j and m_0 is the mass of the bare electron.

We considere a quantum well consisting of $GaAs$ material of width 120 Å and barriers consisting of $Al_yGa_{1-y}As$ with y=0.2237. Both barriers are doped with the δ-potential at

50 Å from the edge of the well. The effective mass of the electrons[11] in the $Al_yGa_{1-y}As$ region for y=0.2237 is 0.08669, whereas in $GaAs$ it is 0.067. The value of y=0.2237 gives a 180 meV potential height.[11] For the undoped structure, there are three states at 21.7, 85.0 and 173.3 meV. Figure 1 shows the normalized wavefunctions of the first four stationary states along with the potential profile in eV for a -4 eVÅ strength of the δ-potential. The situation of the *fourth* bound state is discussed below. It is clear that the probabilities of all the states are greater in the barrier regions in comparison with the undoped structure, are mainly localized in the δ-potential regions, and most of all, are symmetric around the middle of the barrier because the strength of the δ-potentials in both barriers are the same. (The term symmetric means that the probabilities to find an electron in both barrier regions are equal but the parities of the states are conserved.) Another feature worth noting at this point is that the *third* state is mostly localized in the barrier regions, i.e., it is bound to the δ-potentials. The ratio of the probabilities[12] in the barrier regions for the *second* and *first* states is enhanced greatly for the doped structures, which favors of an effect called *light-induced drift* predicted earlier.[6]

As mentioned earlier, there are only three bound states for the undoped structures, but beyond a certain strength of the δ-potential, a *fourth* bound state appears. In view of the origin of the *fourth* state, we have plotted the transmission coefficients for the doped structures for the energies above the surface of the well for different values of δ in Fig. 2(a). A virtual state for the undoped structure exists at about 350 meV, whereas the δ-potential creates a virtual state at about 200 meV and moves its energy down as the strength of the negative δ-potential increases. This virtual state becomes stationary beyond a -0.9 eVÅ value of the strength of the δ-potential. All the energies are measured from the bottom of the quantum well.

The frequencies of the allowed transitions ω_{ij} described in Eq. (5) and calculated with the help of the Eq. (1) are plotted in Fig. 2(b). ω_{12} does not change up to about -3.5 eVÅ, and then it drops gradually to zero which means that after a -3.5 eVÅ strength these

two states get closer and closer and finally vanish forever. ω_{14} decreases monotonically from -0.9 eVÅ up to -3.5 eVÅ. For a range of strength of the δ-potential, ω_{14} does not change much. The range of strength for which this plateau is formed is important since most of the observable changes occur in this range, and from now on we will refer this as a "plateau range". When the first two states vanish gradually, the upper two states take their place. This interchange of these states is not identical because the δ-potential creates a phase difference of π over the plateau range. Changes brought in to other two frequencies ω_{23} and ω_{34} by the δ-potential are also shown in Fig. 2(b), which may be important in emission studies or optically populated absorption.

Figure 3 shows the dipole matrix elements in (a) through (c) and the oscillator strengths in (d) through (f) for the allowed transitions as a function of the strength of the δ-potential. The matrix element $z(1 \leftrightarrow 2)$, Fig. (3a), remains constant at -30 Å up to the plateau range, increases in this range and then decreases rapidly. The constant value of $z(1 \leftrightarrow 2)$ up to -3.5 eVÅ, which is close to the matrix element -21.6 Å for a similar transition in the infinite well of width 120 Å, indicates that changes brought in by the δ-potential to the wavefunctions is symmetrical (ignoring parity). The increase in $z(1 \leftrightarrow 2)$ is due to the fact that the *second* state moves down whereas the *first* one remains the same. This range of δ-potential strength is suitable for infrared detectors. The oscillator strength shown in Fig. (3d) goes through a minimum in the plateau range, but only the transitions up to the bottom of this tip are important, since the frequency ω_{12} goes to zero after this point.

There is very interesting activity for the transition $1 \leftrightarrow 4$. $z(1 \leftrightarrow 4)$ in Fig. (3a) is zero up to the plateau range and goes through a smooth maximum in this range. As we have discussed before, the *fourth* state has been brought in from the continuum by the δ-potential but its wavefunction is essentially the same as that of the *first* one. It is the plateau range in which the wavefunction of the *fourth* state goes to the wavefunction of the *second* one with a phase difference of π. Hence, in this range, while the transition to

the *second* state can be used to tailor the transition, a transition to the *fourth* state is also allowed and gives essentially a constant frequency. This transition to the *fourth* state is only allowed in the plateau range since this state takes the place of the *second* one after the plateau range. The matrix elements $z(2 \leftrightarrow 3)$, $z(3 \leftrightarrow 4)$ are shown in Figs. (3b) and (3c) and the corresponding oscillator strengths in Figs. (3e) and (3f). If either of these *second* and *third* states are populated optically, a tailoring of the transition is possible even for a strength up to the plateau range. Moreover, these matrix elements $z(2 \leftrightarrow 3)$ and $z(3 \leftrightarrow 4)$ and corresponding oscillator strengths are useful in emission studies.

In conclusion, we have demonstrated that a tailoring of the optical transition for a suitable frequency is possible by growing negative δ-potentials in the barrier regions of a single quantum well. We have also shown that beyond a certain value of the strength of the δ-potential, the first two states disappear and the upper two take their places with a phase difference of π. If there are not two stationary state available to take the places of the disappearing ones, the δ-potential brings one down from the continuum.

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9. E. F. Schubert, Optical and Quantum Electronics, **22**, 5241 (1990).
10. L. N. Pandey, D. Sahu and T. F. George, Solid State Commun. **72**, 7 (1989). For this calculation, we choose b=-1.
11. The barrier height and effective mass depend on y, the fraction of Al in the layer of $AlGaAs$ forming the barrier. The number of monolayers of $AlGaAs$ and $GaAs$ define the widths of the barrier and well, respectively. The barrier height is calculated by the formula $V_i(eV) = 0.65(1.155y + 0.37y^2)$ and effective mass by $\frac{m^*}{m_o} = 0.067 + 0.088y$, where m_o is the mass of the bare electron. These formulae are given in detail in a phenomenological study by H. J. Lee, L. Y. Juravel, J. C. Woolley and A. J. SpringThorpe, Phys. Rev. B **21**, 659 (1980).

12. The total probabilities of the electrons in both barriers together for each of the first four states are 0.036, 0.503, 0.98 and 0.611 for a -4 eVÅ δ-potential strength, whereas these probabilities for the first three states of an undoped structure are 0.031, 0.137, and 0.556. Since the *fourth* state becomes stationary at a -0.9 eVÅ δ-potential strength, the probability at that strength for the *fourth* in is 0.889.

Figure Captions

Fig. 1. Energies in eV and wavefunctions of the first four stationary states of a quantum well of width 120 Å and height 180 meV. Both barriers are doped by negative δ-potentials of strength -4 eVÅ at 50 Å from the edge of the well. The potential profile and stationary states are also shown in eV.

Fig. 2. (a): Transmission coefficient as a function of the energy above the surface of the well for different δ-potential strengths.

(b): Frequencies of the allowed transitions as a function of the strength of the δ-potential.

Fig. 3. Matrix elements in (a) through (c) and corresponding oscillator strengths in (d) through (f) of the allowed transitions as a function of the strength of the δ-potential.

Fig. 1 of 3
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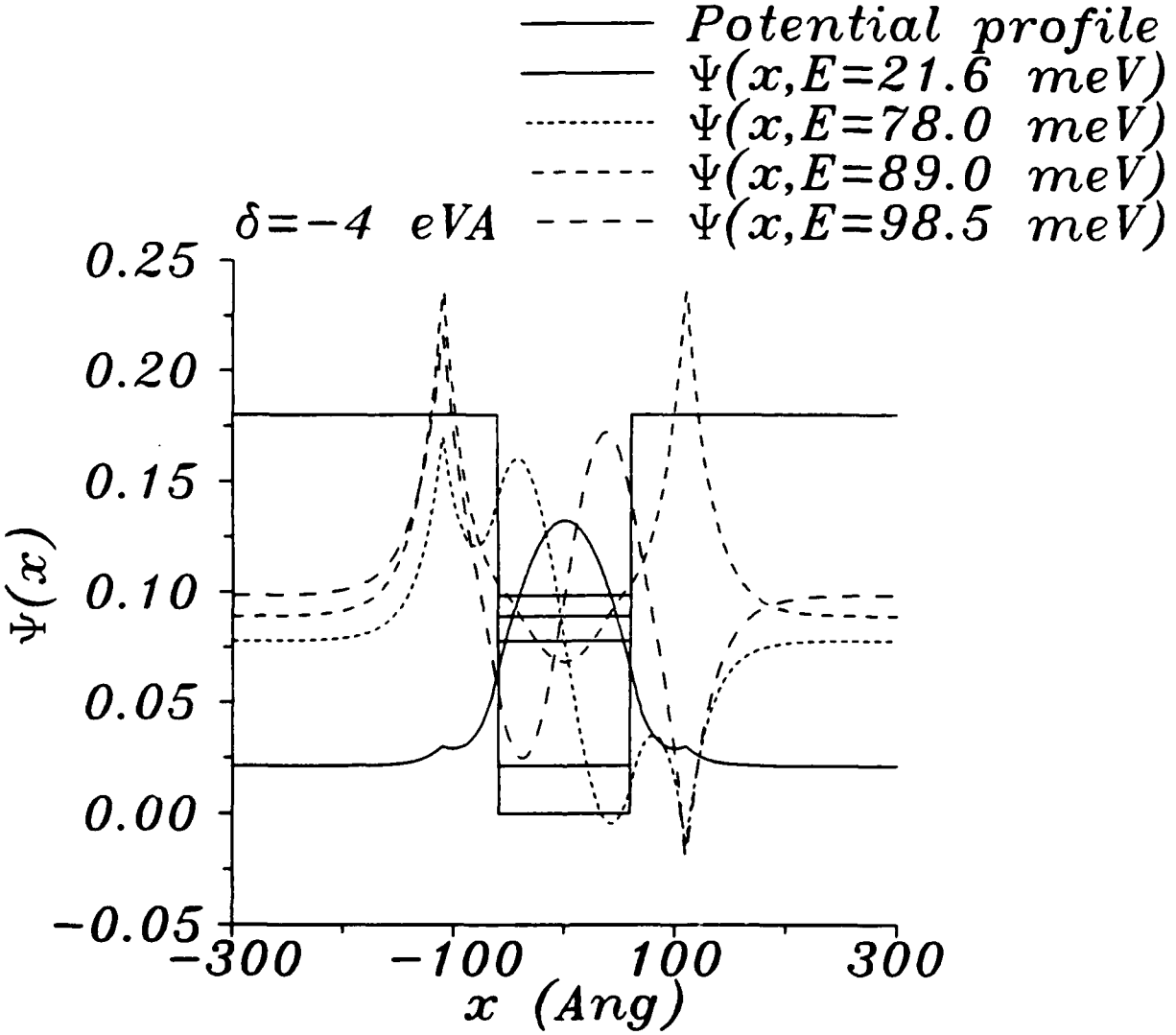

Fig. 2 & 3
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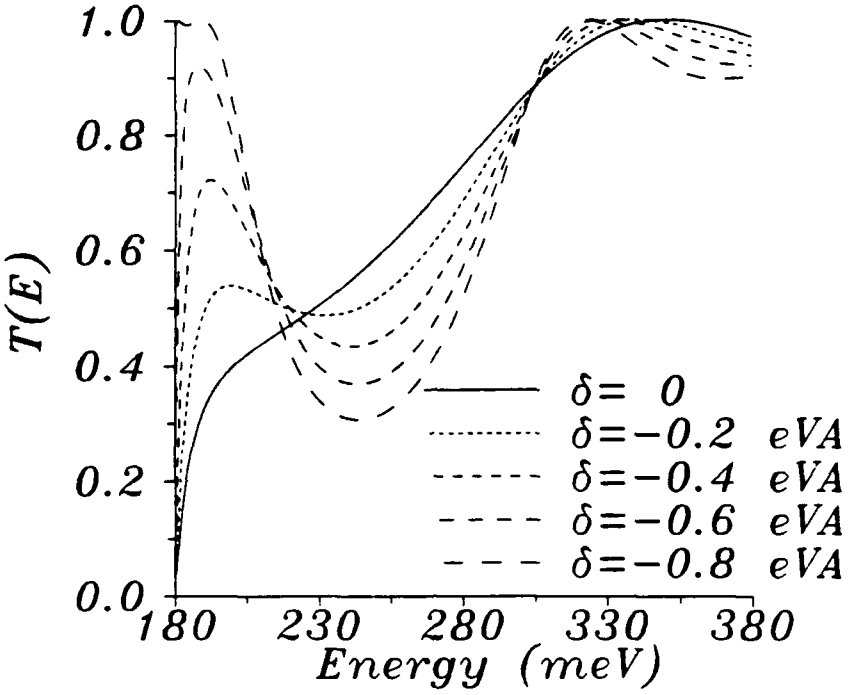
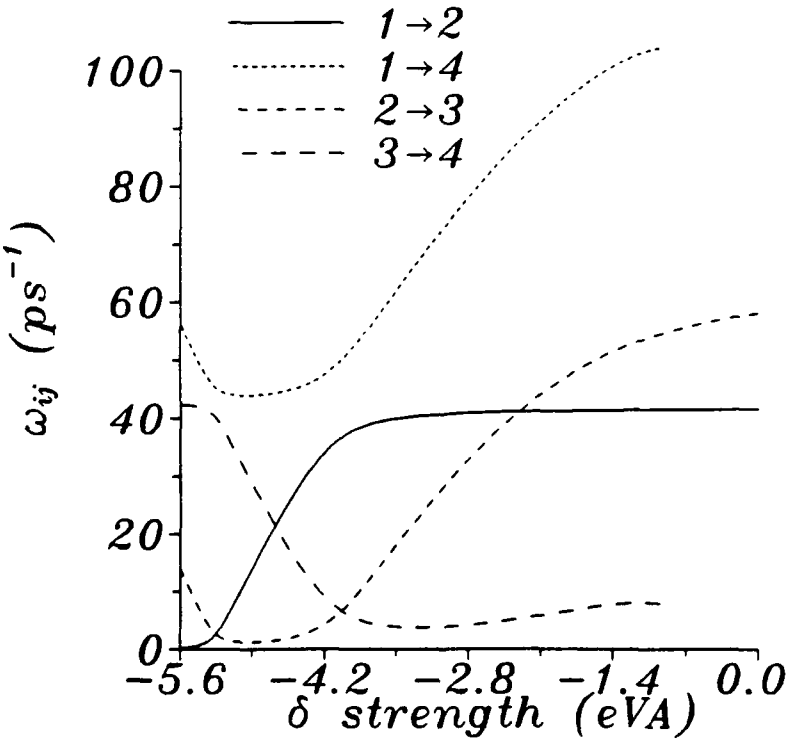
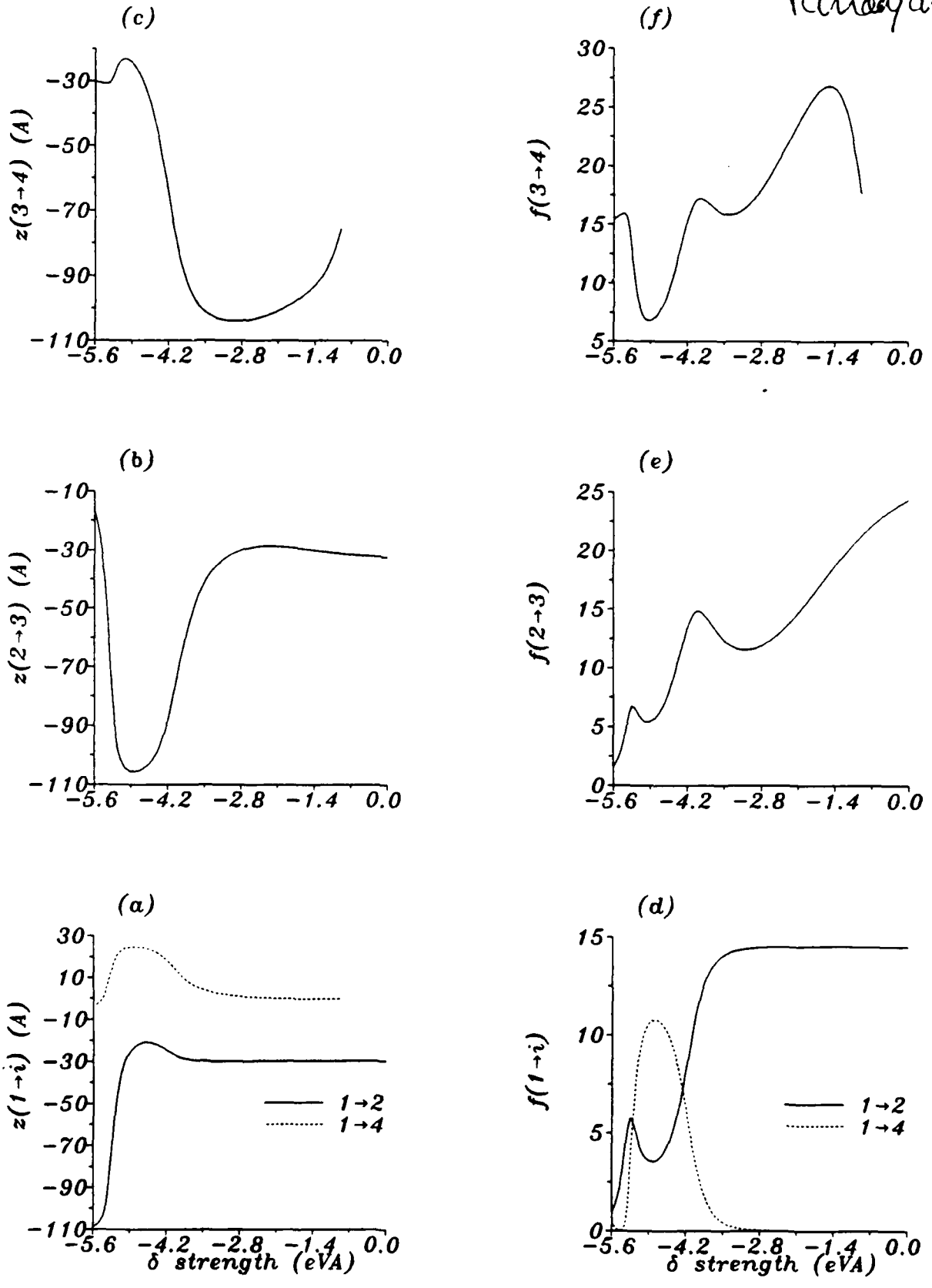
(a)



(b)




(c)
z(3→4) (A)
-30
-50
-70
-90
-110
-5.6 -4.2 -2.8 -1.4 0.0
(f)
f(3→4)
30
25
20
15
10
5
-5.6 -4.2 -2.8 -1.4 0.0
(b)
z(2→3) (A)
-10
-30
-50
-70
-90
-110
-5.6 -4.2 -2.8 -1.4 0.0
(e)
f(2→3)
25
20
15
10
5
0
-5.6 -4.2 -2.8 -1.4 0.0
(a)
z(1→i) (A)
30
10
-10
-30
-50
-70
-90
-110
1→2
1→4
-5.6 -4.2 -2.8 -1.4 0.0
δ strength (eVA)
(d)
f(1→i)
15
10
5
0
1→2
1→4
-5.6 -4.2 -2.8 -1.4 0.0
δ strength (eVA)